Monitoring the interplay between diffusion and reaction during catalytic conversion in nanoporous materials

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The ability of IR microscopy to distinguish between molecular species during in situ measurements provides excellent conditions for the investigation of chemical reactions. The investigated model reaction is the hydrogenation of benzene to cyclohexane in a porous glass membrane as catalyst support for nickel nanoparticles with top and bottom faces sealed by a gas-tight coating [1]. Fig. 1 introduces the measurement procedure. The major advantage of this approach to study catalytic reactions is the direct access to important diffusion and reaction properties. For example, diffusion coefficients, reaction rate constants and effectiveness factors can be directly obtained from the concentration profiles of reactant and product in one single experiment.

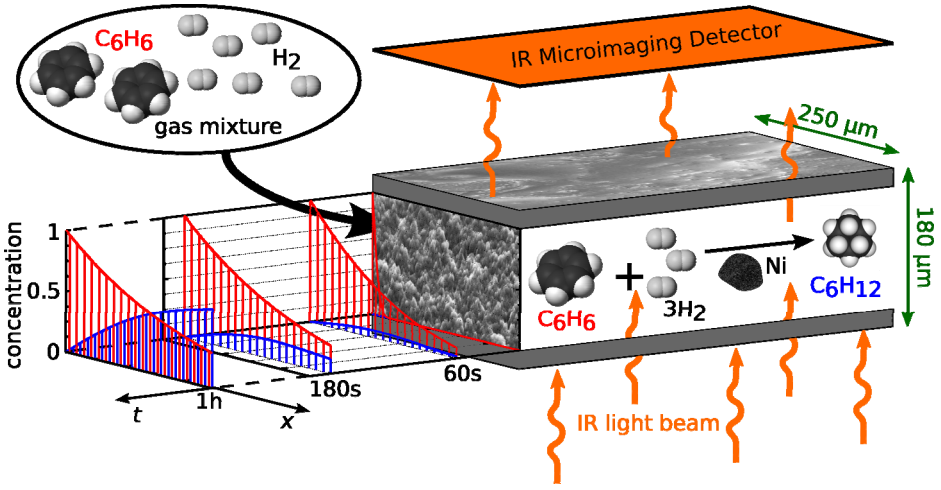

Figure 1: Measurement procedure

The hydrogenation is initiated by bringing a benzene-hydrogen atmosphere into contact with the initially empty catalyst. The local concentrations of benzene (reactant) and cyclohexane (product) are recorded simultaneously by means of IR microimaging. Examples of the resulting time- and space-resolved concentration profiles for both benzene (red) and cyclohexane (blue) are shown on the left. Benzene is seen to propagate into the interior of the catalyst particle forming a well-shaped propagation front. This process is accompanied by the appearance of cyclohexane, emerging as a result of benzene hydrogenation. Benzene concentrations are seen to decay towards the particle interior, indicating benzene influx. Cyclohexane concentration, in contrast, decreases towards the particle boundary, indicating efflux. Both profiles approach a steady state in which the cyclohexane efflux is compensated by the benzene-to-cyclohexane conversion rate.

References

[1] T. Titze, C. Chmelik, J. Kullmann, L. Prager, E. Miersemann, R. Gläser, D. Enke, J. Weitkamp, J. Kärger: *Microimaging of Transient Concentration Profiles of Reactant and Product Molecules during Catalytic Conversion in Nanoporous Materials.* Angew. Chem. Int. Ed. **54**, 5060–5064 (2015).